Mori-Zwanzig formalism

The aim of the problem is to show how so called "generalized Langevin equations" may formally be obtained from a deterministic evolutions by eliminating "irrelevant" degrees of freedom . The procedure is commonly refered to as the "Mori-Zwanzig projection formalism".

Extensive treatment can be found in Zwanzig's book "Non-Equilibrium Statistical Mechanics", 2001 (Chapter 8)

1. A motivational example

Consider the following linear deterministic dynamics in $\mathbb{R}^2$

$$\begin{aligned} \dot{a}_1 &= L_{11}a_1 + L_{12}a_2 \\ \dot{a}_2 &= L_{21}a_1 + L_{22}a_2 \end{aligned} \tag{1}$$

We assume that a_2 is an "irrelevant" variable, so that one wants to get a closed equation for a_1.

Show that a_1 satisfies an equation of the form

$$\dot{a}_1 = L_{11}a_1 + \eta(t) - \int_0^t ds\, K(t-s)a_1(s)$$

where the "noise" term is $\eta(t) := L_{12}e^{L_{22}t}a_2(0)$ and the memory kernel is $K(\tau) = -L_{12}L_{21}e^{L_{22}\tau}$ Please observe that the effective dynamics is closed but clearly non-Markovian. This is the price to pay for eliminating variables !

2. General formalism

We now generalize this observation to a more general, yet slightly abstract, framework. The dynamics is now prescribed by an autonomous ordinary differential equation

$$\dot{\mathbf{x}} = \mathbf{q}(\mathbf{x}) \tag{2}$$

with any choice of a sufficiently smooth function $\mathbf{q} : \mathbb{R}^n \to \mathbb{R}^n$ that guarantees existence and uniqueness of the solutions.

1) Let $\mathbf{x}(t;\mathbf{x}_0)$ denote the solution of (2) for the intial condition $\mathbf{x}(0) = \mathbf{x}_0$. Explain why uniqueness of solutions of this initial-value problem implies that

$$\mathbf{x}(t+s;\mathbf{x}_0) = \mathbf{x}(t;\mathbf{x}(s,\mathbf{x}_0)). \tag{3}$$

2) Use the relation in part (1) to show that

$$\mathbf{q}(\mathbf{x}(t;\mathbf{x}_0)) = \mathbf{q}(\mathbf{x}_0) \cdot \nabla_{\mathbf{x}_0}\mathbf{x}(t;\mathbf{x}_0) \tag{4}$$

Hint: Differentiate both sides with respect to s.

3) Use the relation in part (2) to show that the ODE (2) is equivalent to the linear PDE

$$\partial_t \mathbf{x}(t;\mathbf{x}_0) = \mathbf{q}(\mathbf{x}_0) \cdot \nabla_{\mathbf{x}_0}\mathbf{x}(t;\mathbf{x}_0) \equiv \mathcal{L}\mathbf{x}(t;\mathbf{x}_0) \tag{5}$$

where we defined the 1st-order linear operator $\mathcal{L} = \mathbf{q}(\mathbf{x}_0) \cdot \nabla_{\mathbf{x}_0}$.

4) Suppose that A is a smooth function of $\mathbf{x}$, representing some property of the dynamical system with state $\mathbf{x}$. The time-dependent function $A(t)$ is defined by $A(t;\mathbf{x}_0) \equiv A(\mathbf{x}(t;\mathbf{x}_0))$, with fixed state $\mathbf{x}_0$. Show that

$$\frac{d}{dt}A(t) = \mathcal{L}A(t). \tag{6}$$

5) Suppose that $\mathbf{A} = (A_1, \dots, A_n)$ is a finite set of observables such as in part (4) and define, in the space of observables, the projection operator $\mathcal{P}$ onto the space spanned by the A_i's. Assume (for simplicity) that the elements of $\mathbf{A}$ are orthogonal with respect to the inner-product $\langle C, B\rangle = \int C(\mathbf{x})B(\mathbf{x})\mathrm{d}\mu(\mathbf{x})$ for some probability measure μ on the state space. Then

$$\mathcal{P}B = \sum_{i=1}^{N} A_i \frac{\langle A_i, B\rangle}{\langle A_i, A_i\rangle}. \tag{7}$$

If $\mathcal{Q} = I - \mathcal{P}$, show that $\mathcal{Q}B$ is uncorrelated with all of the A_i's, i.e.

$$\int A_i(\mathbf{x})\mathcal{Q}B(\mathbf{x})\mathrm{d}\mu(\mathbf{x}) = 0. \tag{8}$$

6) Show by differentiating with respect to t that

$$e^{t\mathcal{L}} = e^{t\mathcal{Q}\mathcal{L}} + \int_0^t \mathrm{d}s\, e^{(t-s)\mathcal{L}}\mathcal{P}\mathcal{L}e^{s\mathcal{Q}\mathcal{L}}. \tag{9}$$

7) Write the right hand side of (6) as $\mathcal{L}\mathbf{A}(t) = e^{t\mathcal{L}}\mathcal{L}\mathbf{A} = e^{t\mathcal{L}}(\mathcal{P}+\mathcal{Q})\mathcal{L}\mathbf{A}$ and then use the formula in part (6) to derive a "generalized Langevin equation"

$$\frac{d}{dt}\mathbf{A}(t) = e^{t\mathcal{L}}\mathcal{P}\mathcal{L}\mathbf{A} + \int_0^t \mathrm{d}s\, e^{(t-s)\mathcal{L}}\mathcal{P}\mathcal{L}e^{s\mathcal{Q}\mathcal{L}}\mathcal{Q}\mathcal{L}\mathbf{A} + e^{t\mathcal{Q}\mathcal{L}}\mathcal{Q}\mathcal{L}\mathbf{A}. \tag{10}$$

8) The terms on the righthand-side of equation (10) represent resolved dynamics, a memory term, and a noise term respectively. In particular, show that

$$e^{t\mathcal{L}}\mathcal{P}\mathcal{L}A_i = \sum_{j=1}^{N} L_{ij}A_j(t), \qquad \text{with } L_{ij} := \frac{\langle A_j, \mathcal{L}A_i\rangle}{\langle A_i, A_j\rangle}, \tag{11}$$

,

$$e^{(t-s)\mathcal{L}}\mathcal{P}\mathcal{L}e^{s\mathcal{Q}\mathcal{L}}\mathcal{Q}\mathcal{L}A_i = -\sum_{j=1}^{N} K_{ij}(s)A_j(t-s), \qquad \text{with } K_{ij}(s) := -\frac{\langle A_j, \mathcal{L}F_i(s)\rangle}{\langle A_i, A_j\rangle}, \tag{12}$$

and $\mathbf{F}(t) := e^{t\mathcal{Q}\mathcal{L}}\mathcal{Q}\mathcal{L}\mathbf{A}$ a force uncorrelated to the A_i's.

Show that the equation (10) can then be formally written as

$$\frac{d}{dt}\mathbf{A}(t) = \mathbf{L}\mathbf{A}(t) - \int_0^t \mathrm{d}s\, \mathbf{K}(s)\mathbf{A}(t-s) + \mathbf{F}(t). \tag{13}$$

9) If we regard $\mathbf{F}(t)$ as a noise, and the memory term as a "generalized friction term", Equation 13 can be interpreted as a "generalized Langevin equation". Show that if $\mathbf{K}(s) = \mathbf{K}_0 e^{-\alpha|s|}$, one formally retrieves a standard Langevin equation in the limit $\alpha \to \infty$.